

PHYS6350 Final exam
Due Dec 12 by 12pm

Please note that any requests for an extension on this exam must be accompanied by justification in accordance with university policy (e.g. statement from the Center for Students with Disabilities, a doctor's not explaining the need for an extension, etc.). This is a stricter condition than has been applied to the homework. Also, note the exam is 2 pages (in case you print 2-sided, turn it over before submitting).

On this exam, you are free to use any code we have covered through the course, any function defined in matlab, any library defined in python, and any library in C++'s STL. You are free to use any book, web search, video, and any other resource you feel might be useful. You may use any code provided in class, or in the textbook, or your own homework. You are not permitted to copy solutions or borrow code from one another on this exam, and are not allowed to directly copy and paste code from the internet.

1. **25 points** A Fokker-Plank equation describes the diffusion of a particle in a potential $U(x)$, with

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} + \frac{1}{\zeta} \frac{\partial}{\partial x} \left(n \frac{\partial U}{\partial x} \right) \quad (1)$$

For $U(x) = -fx$, with reflecting boundary conditions at $x = \pm L/2$, analytically determine the steady state solution for $n_\infty(x)$. Numerically integrate the Fokker Plank equation using any method you choose (for any nonzero ζ and f you choose), and show that your predicted steady state solution is recovered as $t \rightarrow \infty$.

2. **30 points** Numerically solve for the wavefunction of a particle approaching a δ function potential, satisfying

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + u\delta(x)\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (2)$$

with the natural units $\hbar = m = 1$, using a Crank-Nichelson scheme. Use the periodic boundary condition $\psi(-L/2) = \psi(L/2)$ for $L = 1000$ (in dimensionless units), and take the initial condition to be a traveling Gaussian packet $\psi(x, 0) \propto e^{ipx/\hbar - (x-x_0)^2/2\sigma^2}$ representing a particle moving towards the δ function barrier with momentum p . You should use $x_0 = -L/4$, $p = 1$, and $\sigma = 20$ (all in dimensionless units). Show that for $u = 0.5$ and $u = 2.0$ the wavepacket is partially transmitted and partially reflected. Numerically compute the amplitude of the transmitted and reflected packets for $u = 0.5$ and 2.0 .

3. **45 points** In this problem you will simulate the dynamics of a 2D Ising model, with Hamiltonian $\beta H = -J \sum_{\langle ij \rangle} s_i s_j$. In all problems, you should simulate a square system of $N = 50 \times 50$ on a square lattice, using periodic boundary conditions. All simulations should include 5×10^5 iterations, and include 100 runs per simulation.

- (a) Starting from a random initial state (50% spins up, and 50% spins down), plot the average energy as a function of time for $J = 0.1, 0.2, 0.3$, and 0.4 . Plot the energy as a function of the iteration number n , $\langle E_n \rangle$, as well as the fluctuations in the energy, $\langle E_n^2 \rangle - \langle E \rangle^2$. Do the fluctuations depend significantly on n and/or J ?
- (b) Fit your simulation result to a single exponential curve, $\langle E_n \rangle = Ae^{-n/\tau_e} + B$, with τ_e the equilibration ‘time’ (use A , B , and τ_e as fitting parameters). What are the values of τ_e you find? Are they constant, or do they vary with J ?
- (c) In (a), you should have found the single exponentially decay doesn’t fit well for all of the curves. Does a bi-exponential fit, $\langle E_n \rangle = Ae^{-n/m_1} + Be^{-n/m_2}$ better fit the data?
- (d) In (b-c), you should have found equilibration on a timescale $\tau_e \lesssim 10^4$ for most of the simulations. For the same values of J , take $\tau_e = 10^4$ and compute $C(n) = \langle m_{\tau_e} m_{n+\tau_e} \rangle$, the correlation between magnetization at two different times at equilibrium. Fit these to an exponential decay, $C(n) = De^{-n/\tau_c}$ with D and τ_c fitting parameters. Are the equilibration times from (b) the same as the correlation times you found here?
- (e) Compute the mean $\langle m \rangle$ and standard deviation of the mean $\sigma_m = (\langle m^2 \rangle - \langle m \rangle^2)/\sqrt{n_{run}}$ for $J = 0.1, 0.2$, and 0.3 using the procedure described in class: discard the equilibration data and sampling the data at a rate inversely proportional to the correlation time.